Chapter 17 - GRAVITY CORRECTING PRISMS

Prisms are used to deflect the neutron beam upward thereby correcting for neutron fall due to gravity at long wavelengths. Prisms contribution to SANS resolution and Q_{min} are discussed here (Hammouda-Mildner, 2007).

1. NEUTRON TRAJECTORY

The parabolic neutron trajectory equation in the pre-sample collimation follows.

$$\mathbf{y}(\mathbf{z}) = \mathbf{B}\lambda^2 \mathbf{z}(\mathbf{L}_1 - \mathbf{z}) \qquad 0 \le \mathbf{z} \le \mathbf{L}_1 \tag{1}$$

with:

$$B = \frac{gm^2}{2h^2} = 3.073 * 10^{-9} \text{ cm}^{-1} \text{Å}^{-2}.$$
 (2)

The z-direction is along the neutron beam and the y axis is in the vertical direction. L_1 is the source-to-sample distance. The vertical component of the neutron trajectory slope y'(z) is therefore:

$$y'(z) = B\lambda^{2}(L_{1} - 2z)$$
 $0 \le z \le L_{1}$ (3)
 $y'(L_{1}) = -B\lambda^{2}L_{1}$ $z = L_{1}$.

This neutron trajectory holds between the sample and detector. The addition of a prism changes the neutron trajectory by introducing an upward deflection of angle δ .

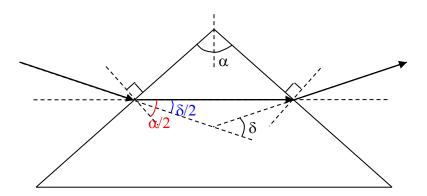


Figure 1: Schematics of a prism showing the deflected neutron trajectory in the simple case of minimum deviation.

The slope of the neutron trajectory is changed to

$$y'(L_1) = -B\lambda^2 L_1 + \delta$$
 $z = L_1.$ (4)

The neutron trajectory is therefore changed between the sample and detector to the following form:

$$\begin{split} y(z) &= -B\lambda^2(z-L_1)^2 + [-B\lambda^2L_1 + \delta](z-L_1) & L_1 \leq z \leq L_1 + L_2. \\ y(L_1 + L_2) &= -B\lambda^2L_2(L_1 + L_2) + \delta L_2 & z = L_1 + L_2. \end{split} \tag{5}$$

The use of a prism with deflection angle $\delta = B\lambda^2(L_1+L_2)$ would correct for the gravity effect exactly.

2. THE PRISM DEFLECTION ANGLE

The "prism equation" (case of minimum deflection where the refracted beam is parallel to the prism base) relates the deflection angle δ , the prism angle α and the index of refraction n as:

$$n = \frac{\sin\left(\frac{\alpha - \delta}{2}\right)}{\sin\left(\frac{\alpha}{2}\right)}.$$
 (6)

This is the Snell's law of refraction (also referred to as the Descartes law). The deflection angle is expressed as:

$$\delta = \alpha - 2\sin^{-1} \left[n \sin \left(\frac{\alpha}{2} \right) \right]. \tag{7}$$

The wavelength dependence of the deflection angle enters through the index of refraction.

$$n = 1 - \frac{\rho b_c}{2\pi} \lambda^2. \tag{8}$$

For MgF₂ prisms, $\rho b/\pi = 1.632*10^{-6}$ Å⁻² so that $n = 1-0.816*10^{-6}\lambda^2$ (where λ is the neutron wavelength in Å).

In the small deviation angle approximation, one can expand the prism formula with $\delta << \alpha$ to obtain:

$$\delta(\lambda) \cong \left(\frac{\rho b}{\pi}\right) \tan\left(\frac{\alpha}{2}\right) \lambda^2 = C\lambda^2. \tag{9}$$

This is an easier (approximate) expression to use in order to obtain analytical results.

3. CONTRIBUTION TO THE Q RESOLUTION

The Q resolution at the detector (where $z = L_1 + L_2$) involves the spatial variance σ_y^2 .

$$\sigma_{y}^{2} = \left[\sigma_{y}^{2}\right]_{geo} + \langle y(L_{1} + L_{2})^{2} \rangle - \langle y(L_{1} + L_{2}) \rangle^{2}$$
 (10)

$$y(L_1 + L_2) = -B\lambda^2 L_2(L_1 + L_2) + \delta(\lambda)L_2.$$
 $z = L_1 + L_2$

With the deviation angle given by $\delta(\lambda) = C\lambda^2$, where C depends on the prism material and apex angle the following result is obtained.

$$\sigma_{y}^{2} = \left[\sigma_{y}^{2}\right]_{geo} + \left[A - L_{2}C\right]^{2} \left[\langle \lambda^{4} \rangle - \langle \lambda^{2} \rangle^{2}\right]. \tag{11}$$

Here the gravity variable $A = BL_2(L_1+L_2)$ has been used.

Assuming a triangular wavelength distribution, the wavelength averages are calculated as follows:

$$[\langle \lambda^4 \rangle - \langle \lambda^2 \rangle^2] = \lambda^4 \frac{2}{3} \left(\frac{\Delta \lambda}{\lambda}\right)^2. \tag{12}$$

Therefore:

$$\sigma_y^2 = \left[\sigma_y^2\right]_{geo} + \left[A - L_2C\right]^2 \lambda^4 \frac{2}{3} \left(\frac{\Delta \lambda}{\lambda}\right)^2$$
 (13)

This is the variance of the neutron spot spatial resolution at the detector in the vertical direction. By analogy, the case without prisms is obtained for C = 0. The familiar "geometry" contribution is given in terms of the source aperture radius R_1 , sample aperture radius R_2 and detector cell size Δy_3 .

$$\left[\sigma_{y}^{2}\right]_{geo} = \left(\frac{L_{2}}{L_{1}}\right)^{2} \frac{R_{1}^{2}}{4} + \left(\frac{L_{1} + L_{2}}{L_{1}}\right)^{2} \frac{R_{2}^{2}}{4} + \frac{\Delta y_{3}^{2}}{12}$$
(14)

Since most often $\Delta x_3 = \Delta y_3$, $[\sigma_x^2]_{geo} = [\sigma_y^2]_{geo}$. The standard deviation of the Q resolution σ_{Qy} is related to the spatial standard deviation σ_y as $\sigma_{Qy} = \left(\frac{2\pi}{\lambda L_2}\right)\sigma_y$.

4. CONTRIBUTION TO OMIN

Q_{min} has contributions from geometry, gravity effect and the addition of a prism.

$$Y_{\min} = \left[Y_{\min}\right]_{geo} + \left|A - L_2C\right| \frac{\left[(\lambda + \Delta\lambda)^2 - (\lambda - \Delta\lambda)^2\right]}{2}.$$
 (15)

The wavelength term can be expressed (to first order) as:

$$\frac{\left[(\lambda + \Delta\lambda)^2 - (\lambda - \Delta\lambda)^2\right]}{2} \cong 2\lambda^2 \left(\frac{\Delta\lambda}{\lambda}\right) \tag{16}$$

Therefore:

$$\mathbf{Y}_{\min} = \frac{\mathbf{L}_2}{\mathbf{L}_1} \mathbf{R}_1 + \frac{\mathbf{L}_1 + \mathbf{L}_2}{\mathbf{L}_1} \mathbf{R}_2 + \frac{\Delta \mathbf{y}_3}{2} + |\mathbf{A} - \mathbf{L}_2 \mathbf{C}| 2\lambda^2 \left(\frac{\Delta \lambda}{\lambda}\right). \tag{17}$$

Note that the same factor $|A-L_2C|$ enters in the resolution variance σ_y^2 and in Y_{min} . Q_{ymin} is obtained by multiplying Y_{min} by the factor $(2\pi/\lambda L_2)$.

5. MEASUREMENTS WITH GRAVITY CORRECTING PRISMS

A prism cassette containing a row of five prisms is used for neutron optics measurements. Each prism is made out of single-crystal MgF₂ and has a base of 3 cm*3 cm and a height of 0.5 cm. In order to correct fully for the effect of gravity, between one and two prism cassettes would have to be used. Here only one cassette is used for the sake of simplicity.

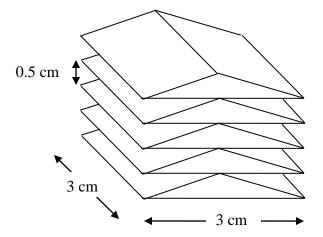


Figure 2: Representation of the prism cassette containing a row of 5 MgF₂ prisms.

The prism angle is equal to $\alpha = 2 tan^{-1}(1.5/0.5) = 143.13^{\circ}$. The prism variable is $C = 4.896*10^{-6} \text{ Å}^{-2}$ yielding an estimate for the factor $L_2C = 6.458*10^{-3} \text{ cm.Å}^{-2}$ and for the factor $|A - L_2C| = 0.00543 \text{ cm/Å}^2$.

A set of neutron optics measurements have been performed using the following instrument configuration:

$$L_{1} = 16.14 \text{ m}$$

$$L_{2} = 13.19 \text{ m}$$

$$R_{1} = 0.715 \text{ cm}$$

$$R_{2} = 0.635 \text{ cm}$$

$$\Delta x_{3} = \Delta y_{3} = 0.5 \text{ cm}$$

$$\frac{\Delta \lambda}{\lambda} = 0.13.$$
(18)

This gives A = 0.01189 cm/ \mathring{A}^2 .

The vertical position of the neutron beam varies with the neutron wavelength I following the parabola:

$$y(L_1 + L_2) = (-A + L_2C)\lambda^2$$
 $z = L_1 + L_2$ (19)

When no prisms are used (C = 0), neutrons fall due to gravity. When prisms are used, falling neutrons are deflected upward. This is plotted as a function of wavelength and compared to the measured values. The value corresponding to $\lambda = 6$ Å has been subtracted in each case for simplicity.

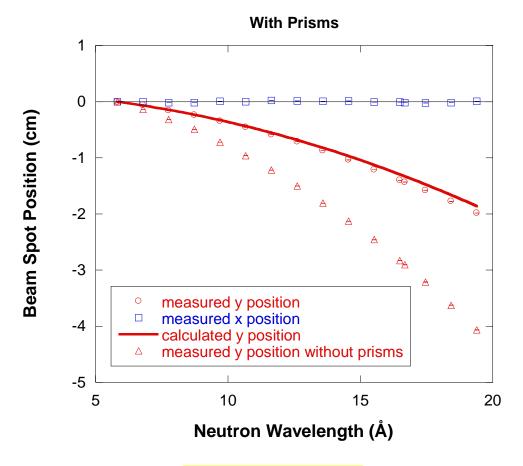


Figure 3: Variation of the neutron beam spot positions with wavelength. Statistical error bars are smaller than the plotting symbols.

The variance of the neutron beam spot at the detector has also been measured in each case and compared to the calculated value. A figure shows the square root of the difference in the variances of the beam spot in the orthogonal directions as a function of wavelength. The measured values are obtained using the same procedure described in previous chapters (taking horizontal and vertical slice cuts across the neutron beam spot). The prediction for the case without prisms is also shown. The measured values are seen to be systematically higher than the calculated ones. This is believed to be caused principally by neutrons leaking between the apex and the base of adjacent prisms.

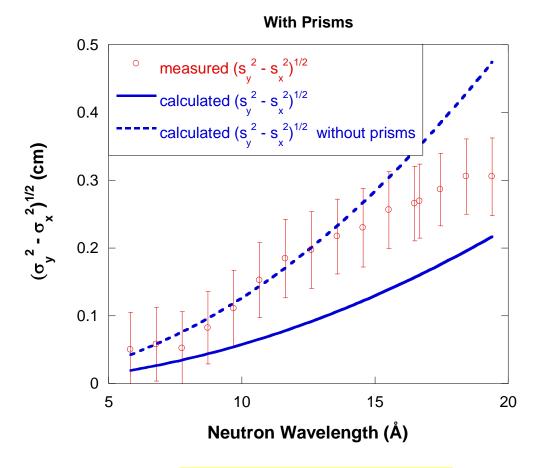


Figure 4: Variation of the variance of the neutron spot at the detector with wavelength. Statistical error bars have been included. Discrepancy between measured and calculated values is likely due to neutron leakage between adjacent prisms.

6. PRISMS TRANSMISSION

Consider a prism system containing a row of prisms of width W and height H and assume a beam defining aperture of radius B.

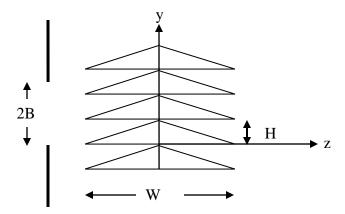


Figure 5: Transmission through one row of prisms.

The transmission through one row of prisms using a source aperture of diameter $2R_2$ can be calculated as follows.

$$T = \frac{\int_{0}^{2B} dy \exp\left[-\Sigma_{t} 2z\right]}{2B}$$
 (20)

Here 2z is the path across a prism at a height y. For $0 \le y \le H$, it is 2z = (H-y)W/H. The integration is performed for y covering each prism. When 2B is not a multiple of H, the result is:

$$T = \frac{[2 - 3\exp(-\Sigma_{t}W) + \exp(-3\Sigma_{t}W + \Sigma_{t}2BW/H)]}{\Sigma_{t}2BW/H}$$
 (21)

Note that this expression is for the transmission of one row of prisms. When 2B is a multiple of H, T is given simply by T_m :

$$T_{m} = \frac{[1 - \exp(-\Sigma_{t} \mathbf{W})]}{\Sigma_{t} \mathbf{W}}$$
 (22)

This result assumes that the beam defining aperture is rectangular. The total cross section for MgF₂ is estimated empirically as Σ_t (cm⁻¹) = 0.00513 λ (Å). A transmission measurement of the cassette containing two rows of prisms has been made using a sample aperture of 2B = 1.27 cm and a neutron wavelength of λ = 17.2 Å. The measured transmission was found to be T = 0.70 while the predicted transmission is T = 0.75. This result is not reliable due to the neutron streaming in-between the prisms.

7. DISCUSSION

Prisms correct for the neutron fall by deflecting the direct neutron beam back up. They also correct for the anisotropy of the neutron beam spot on the detector. Gravity deforms this spot to an oval shape. Prisms correct this shape back to a circular shape. Analytical expressions for the spatial resolution have been presented. Neutron beam optics measurements using a prism cassette have been made. Good agreement was found between calculated and measured beam spot positions. However, no good agreement was found for the instrumental resolution variance due to neutron leakage between adjacent prisms.

REFERENCE

B. Hammouda and D.F.R. Mildner, "SANS Resolution with Refractive Optics", J. Appl. Cryst. 40, 250-259 (2007).

QUESTIONS

- 1. What is the advantage of using prisms in neutron optics?
- 2. Prisms refract incident white light into what?
- 3. The use of gravity correcting prisms affects what part of the instrumental resolution variance?
- 4. What is the wavelength dependence of the prism deflection angle?
- 5. What is the prisms minimum deviation approximation?
- 6. Could a prism system be used for all neutron wavelengths?

ANSWERS

- 1. Prisms correct for gravity effects. At long wavelengths the effect of neutron fall (due to gravity) is to lower the neutron beam spot and deform it into an oval shape. The use of prisms kicks the neutron spot back up and corrects it back to a circular shape.
- 2. Prisms refract incident white light into the rainbow spectrum.
- 3. The use of gravity correcting prisms affects the wavelength spread part of the instrumental resolution variance.
- 4. The prism deflection angle varies like the square of the wavelength.
- 5. The prism's minimum deviation approximation corresponds to the case where the refracted beam (inside the prism) is parallel to the prism's base.
- 6. Since the gravity correction factor (A- L_2 C) is independent of neutron wavelength λ , the same prism system can be used to correct for gravity at all wavelengths.